Hexachloroethane

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 203 °C

Global applicability domain: Inside

Local applicability domain index: 6.70e-01

Confidence level: 7.56e-01

Nearest Neighbors from the Training Set

Image not found
1,1,1,2,3-Pentachloropropane
Measured: 180
Predicted: 190

Image not found
Propane, 1,1,2,3,3-pentachloro-
Measured: 199
Predicted: 196

Image not found
Propane, 1,1,1,3,3,3-hexachloro-
Measured: 206
Predicted: 210

Image not found
Pentane,1,5-dibromo-
Measured: 222
Predicted: 211